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Inventory of aqueous and sediment-associated organic pollutants released by the 2021 flood in the Vicht–Inde catchment, Germany

Piero Bellanova^{1*}, Jan Schwarzbauer² and Klaus Reicherter¹

Abstract

Background The European flood that occurred between July 13th and 16th 2021, was a natural disaster that caused significant damage in Central European countries, including Germany, Netherlands, Belgium, and Luxembourg. This disaster resulted in the highest number of fatalities from a natural disaster in Germany during the twenty-first century, with over 180 people losing their lives and causing damages exceeding 30 bn€. The flood caused severe destruction in small mountainous river systems such as the Vicht and Inde rivers, particularly in the German state of North Rhine-Westphalia. In addition, the flood caused a significant release of pollutants, including old burdens from the former mining area of Stolberg.

Results To assess the extent of pollution caused by the flood in the affected floodplains and urban areas, this study was conducted to inventorize organic contaminants identified through a non-target screening in water and sediment samples taken immediately after the disastrous flood event. In total, 56 individual contaminants were identified from the water samples, including substances derived from urban effluents, such as personal care products, cosmetics, odors, technical additives, pharmaceuticals and surfactants. The analysis of sediment samples revealed different types of environmentally hazardous contaminants, such as petrogenics, urban effluent and wastewater indicators, chlorinated industrial compounds, and pesticides. This diverse range of pollutants and their broad dispersion across various environments in the catchment is attributed to the dynamic nature of the flood.

Conclusion The inventory of identified organic contaminants raises long-term environmental concerns and potential health implications for the flood-affected Vicht–Inde region.

Keywords 2021 flood, Non-target analysis aqueous pollution, Sediment-associated pollution

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Background

In the summer of 2021, the Eifel-Ardennes regions and associated uplands of Germany, Belgium, Luxembourg, and the Netherlands faced one of the most devastating flood disasters in recent history. The period between July 12th and 15th, was exceptional as a meteorological constellation [52, 60] with extreme precipitation (>150 mm/ m^2 , [85]) over a small mountainous region led to unparalleled flooding along the Ahr, Inde, Meuse, and Rur rivers and their tributaries (e.g., Vicht, Wurm, Vesdre, Ourthe).



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The scale and abruptness of the 2021 flood were unprecedented in Germany, with many areas experiencing water levels that surpassed previous records (e.g., [30, 71]). Existing (critical) infrastructure and defenses were overwhelmed, resulting in flood waters sweeping through various smaller and medium-sized cities (e.g., [62]), leaving residents displaced and a trail of destruction in its wake (Fig. 1; e.g., [59, 90]). In contrast to past floods along major river systems (e.g., Elbe, Rhine, Meuse) where water levels rose much more slowly, the events of this flood unfolded rapidly with short warning times.

Major river systems are known to be highways for pollutants with various residence times either within their water phase or associated with sediments transported in the river or archived with high-stand deposits on floodplains (e.g., [7, 103]). In particular, river floods are the main drivers for the release, remobilization, and distribution of organic and inorganic contaminants in the aqueous and sediment phase ([19], and references therein). Regions with a history of anthropogenic pollution can be more severely affected by flood-induced mobilization, including the emission from anthropogenic sources and the (re-)activation of legacy pollution present in the environment, and widespread distribution of contamination, with long-lasting effects on the environment and local communities (e.g., [19]).

Well-documented examples of smaller rivers with a long history of mining-related and industrial pollution that were also affected by the 2021 floods are the Inde and the Vicht (e.g., [110]—this issue). In particular, man-made heavy metal contamination since the Medieval times has been known to pollute the Vicht and Inde catchments (e.g., [28, 87, 92]). The 2021 flood provided unpredictable forces and prompted the remobilization of old burdens and the distribution of heavy metals (Zn, Pb, Cd, Cu, and As) across the inundated floodplains and urban areas of the catchment (e.g., [62, 110]—this issue). In addition, organic contaminants in the aqueous phase or associated with flood sediments have been released (through destruction or flooding), remobilized, and



Fig. 1 Flood damages along the Vicht and Inde rivers. A Damages to the infrastructure and potential pollution sources in Stolberg city center (Rathausstrasse) near the Vicht river. Photo—courtesy of Tristan Lothmann. B Flood damages to the industrial area (near Aurubis Stolberg GmbH & Co.) along the upstream parts of the Vicht river in Stolberg (Zweifaller Strasse). Photo taken by Piero Bellanova. C Household debris a few days after the 2021 flood in Stolberg. Photo—courtesy of Tristan Lothmann. D Floodplain high-stand deposits along the Vicht between Stolberg and Zweifall. Photo—courtesy of Tristan Lothmann

spread across the catchment areas (e.g., [62]). This type of pollution has not been as well-documented as heavy metals in the past. In the wake of such dramatic events as the 2021 flood, research politics, and media focus on recovering and rebuilding the infrastructure. Often, more shrouded questions and the long-term effects of such floods remain unaddressed. However, in times of increasing environmental and pollution-related challenges (e.g., [82]) and the uniqueness of the 2021 flood in Central Europe in scale of destruction pose research questions regarding the presence of organic pollution including emerging contaminants, their release, remobilization, and distribution, as well as ecotoxicological and hazardous effects on local communities and the environment are becoming more pressing issues (e.g., [108]) to be resolved for better preparation and improved societal rehabilitation after inevitable future natural disasters. Therefore, this study aims to (a) inventorize the nonpolar organic pollution derived by the 2021 flood for water and sediment phases in the Vicht-Inde catchment based on a non-target analysis; (b) characterize and provide the pollution profile of different environmental settings affected by the 2021 flood (e.g., floodplains, urban areas, and households); and (c) evaluate and trace pollution sources activated by the flood.

Material and methods

Study area The Inde catch

The Inde catchment (~359 km²) encompasses eight smaller tributary catchments. Among these, the Vicht is by far the most significant tributary with a catchment of 104.2 km² and a traversing length of 23 km directly through the city of Stolberg, at which the northern end of the Vicht and Inde rivers converge (Fig. 2). The catchment area is divided into an upstream confined valley area-particularly evident along the Vicht upstream of Stolberg—and a downstream flatter terrain that stretches along the course of the Inde river to its confluence with the Rur river. This geographical distinction is significant in the context of the 2021 flood, influencing the severity of destruction and the potential release of pollutants. Regions most profoundly impacted by the 2021 flood exhibit distinctive geological attributes, namely shallow soils and topographical characteristics typified by V-shaped notch valleys. These geological and topographic features render the incised river systems, such as the Vicht, particularly susceptible to amplifying effects (e.g., [22, 60, 62]). Physical impact damages are most prevalent along the valley-confined Vicht upstream of the Vicht-Inde confluence. Conversely, in the more level terrain downstream of the Inde river, beginning with the city of Eschweiler, the most prevalent damages are associated with elevated water levels and prolonged ponding beyond the natural floodplains (Fig. 2).

Field survey and sampling

During and in the days and weeks after the 2021 flood (July 15th–October 19th, 2021), several interdisciplinary research parties of RWTH Aachen University dispatched to the affected regions (see other publications of this special issue). For this study, 3 water samples from basements and 12 sediment samples from floodplains, urban areas, and households were collected between July 15th-22nd (Fig. 2, Table 1). Alongside of the sampling, infrastructural damages, eyewitness accounts, flood marks, and distribution of over-wash deposits were documented during the field survey of this study and other studies of this special issue (e.g., [62, 99, 110]). To investigate the flood-related pollutant inventory based on a non-target screening, the samples collected from the study area represent four environments, each characterized by attributes influencing the release, type, and accumulation of pollutants. These pollutant inventories primarily differentiate between those associated with the water phase and sediment-associated contaminants. The latter category can be further subdivided into sediments collected from (1) natural floodplains both upstream (F2) and downstream of urban agglomerations (F1, F3, and F4; Table 1; Fig. 2), as well as floodplains in river restoration zones (F3, F4, and F5); (2) urban sediments in upstream areas predominantly affected by physical damages (e.g., Stolberg, Zweifall, Vicht-U1, U2, U3, and U4); (3) urban sediments in downstream areas primarily impacted by flooding and high water levels (e.g., Eschweiler-U4), and (4) specific households, garages and basements (H1, H2, W1-3) as potential local hotspots. Across all environments, samples have been collected, accompanied by documentation of varying degrees and types of damages, which might be supportive to explain potential variations in pollutant inventory detected.

Water sample extraction

The water samples were collected and extracted using pre-cleaned glass or metal tools to minimize contamination. All solvents used for pre-cleaning and extraction were purchased from Merck, Germany, and distilled over a 0.5-m packed column (reflux ratio approx. 1:25). Gas chromatographic analyses tested solvent purity. To avoid any geochemical alteration, the water samples were extracted immediately after sampling. The water samples underwent filtration through pre-cleaned GF/F filters (Macherey-Nagel, Düren, Germany) to eliminate suspended particulate matter from the aqueous phase. Subsequently, liquid–liquid extraction was performed on water sample aliquots ranging between 0.5 and 1 L.



Fig. 2 A Overview map of the sampling locations along the Vicht–Inde catchment. Blue circles indicate the 3 water samples, green circles indicate the 5 floodplain sediment samples, red circles indicate the 5 urbans sediment samples, and yellow circles indicate the 2 urban-household sediment samples. Grey diamonds show additional sampling locations from the RWTH Aachen University sampling party. Grey areas show urban areas, the brown area shows the lignite mine Inden. **B** 72 h-summarized precipitation map of the areas affected by the 2021 flood. The color code indicates the sum of precipitation in mm. Framed in red is the Vicht–Inde river catchment

The subsequent extraction of water samples was conducted utilizing established and previously documented protocols after Dsikowitzky et al. [24] and Schwanen and Schwarzbauer [91].

Samples were extracted sequentially in a separatory funnel using 50 mL *n*-pentane (fraction 1), 50 mL dichloromethane (DCM, fraction 2), and 50 mL dichloromethane post-acidification to pH 2 (fraction 3). Each fraction was agitated for 5 min then

separated. Subsequently, all fractions were concentrated to approximately 2 mL through rotary evaporation and dried with anhydrous granulated sodium sulfate. Anhydrous granulated Na_2SO_4 and hydrochloric acid were cleaned with pure solvents before usage. The acidic compounds within fraction F3 underwent additional methylation by adding BF₃-methanol. For GC–MS analysis, all fractions were concentrated to final volumes of 10 to 50 µL (F1 and F2) and 200 µL (F3).

Sample	Lab ID	Environment	Description	Latitude	Longitude
Sediment samples					
F1	21/560	Floodplain	Floodplain outside of Zweifall, sediment containing washed out road fill material	50° 43′ 29.42″ N	6° 15′ 32.80″ E
U1	21/461	Urban	Mud sample on the roadside (Eifelstrasse, Vicht)	50° 44′ 41.00″ N	6° 15′ 45.30″ E
U2	21/568	Urban	Sediment from a backyard (Enkereistrasse, Stolberg)	50° 46' 09.96" N	6° 13′ 54.45″ E
H1	21/564	Household	Sample from a basement (Salmstrasse, Stolberg)	50°46′38.53"N	6°13′24.39"E
U3	21/460	Urban	Mud sample on the roadside (corner Eisenbahnstrasse/Heinrich-Heimes-Brücke, Stolberg)	50° 46′ 42.90″ N	6° 13′ 21.20″ E
F2	21/532	Floodplain	Sample from the point bar (corner Haumühle/Talstrasse, Stolberg)	50° 45′ 55.70″ N	6° 12′ 18.30″ E
U4	21/455	Urban	Mud sample on the roadside near the Saint Gobain industrial complex (Eschweilerstrasse, Stolberg)	50° 47′ 26.50″ N	6° 13′ 22.60″ E
U5	21/458	Urban	Mud sample from the parking lot of a shopping center (August-Thyssen-Strasse, Eschweiler)	50° 49' 06.50" N	6° 15′ 45.42″ E
H2	21/592	Household	Sediment trapped in house (Langwahn, Eschweiler)	50° 49′ 10.20″ N	6° 15′ 47.55″ E
F3	21/534	Floodplain	Floodplain sample from the transition zone between straightened section and river restoration section of the Inde river	50° 49' 00.10" N	6° 17′ 57.20″ E
F4	21/527	Floodplain	Sediment sample from the rerouted and near-natural landscape of the "Neue Inde"	50° 52′ 15.60″ N	6° 18′ 34.10″ E
F5	21/523	Floodplain	Sediment sample from the river restoration zone at the Inde–Rur confluence	50° 53′ 53.50″ N	6° 21′ 51.20″ E
Water sar	mples				
W1	21/488	Household	Basement water sample (Grüntalstrasse, Stolberg)	50° 46′ 10.98″ N	6° 13′ 52.50″ E
W2	21/490	Household	Basement water sample (Nothbergstrasse, Eschweiler)	50° 48′ 53.55″ N	6° 16′ 14.96″ E
W3	21/489	Household	Sample pumped out of basement (Nothbergstrasse, Eschweiler)	50° 48' 47.80" N	6° 16′ 36.88″ E

 Table 1
 Information on sampling locations along the Vicht and Inde rivers

Samples originating from household are only listed by street not with a specific address for privacy reasons

Sediment sample extraction

The sediment samples were collected and extracted using pre-cleaned glass or metal tools to minimize contamination. Sediment samples were stored in metal containers at temperature below - 20 °C until extraction was ensured to avoid microbial alteration of the geochemical signature. All solvents used for pre-cleaning and extraction were purchased from Merck, Germany, and distilled over a 0.5-m packed column (reflux ratio approx. 1:25). Gas chromatographic analyses tested solvent purity. Of all sediment samples, 15–20 g aliquots of wet material were mixed with 2 g of diatomaceous earth (Dionex ASE^{TM} Prep DE) and filled in an accelerated solvent extraction cell. Samples were extracted using 30 mL of acetone, acetone/*n*-hexane 1:1, and *n*-hexane, each. The aqueous phase was separated by a surplus of *n*-hexane while volume reduction via rotary evaporation (300 mbar). The reduced extract was dried over a microcolumn filled with anhydrous granulated sodium sulfate and desulphurized with activated copper powder in ultrasonic agitation. Anhydrous granulated Na₂SO₄ and hydrochloric acid were cleaned with pure solvents before usage.

Column chromatography with a microcolumn, filled with 2 g activated silica gel and conditioned at 200 °C, was used to fractionate extracts into 6 fractions (B1–B6) using different mixtures of the eluents *n*-pentane,

dichloromethane (DCM) and methanol (MeOH) (after [9, 94]). Acidic compounds of fraction 6 have been methylated by adding BF_3 -methanol and silylated with acetic anhydride and pyridine.

GC and GC-MS analysis

All sample fractions were measured by gas chromatography–mass spectrometry (GC–MS) to identify organic contaminants. Measurements were performed on a quadrupole, GC–MS instrument (Thermo Finnigan Trace GC/MS) with helium as carrier gas and equipped with a 30 m×0.25 mm i.d.×0.25 µm film ZB-5 fused silica capillary column (Zebron capillary GC column Chrompack). Of each sample fraction, 1 µL was injected at a start temperature of 60 °C with a splitless time of 60 s, a temperature hold of 3 min, followed by a temperature ramp of 3 °C/min to 310 °C and another hold for 20 min. The mass spectrometers operated in full-scan mode, ranges from 35 to 500 *m/z* in positive electron impact ionization mode (EI⁺) with 7 eV.

Individual organic compounds were identified from the non-target screening approach by comparison of EI⁺ mass spectra with those of mass spectral databases (NIST, Wiley) and published information. Furthermore, the identification was verified with mass spectra of purchased reference compounds to consider specific gas chromatographic retention times and elution orders. Pollutant inventories for water and sediment samples were compiled based on compounds that were above the limit of detection (LoD).

Quality assurance and quality control (QA/QC)

Data quality assurance (QA) and quality control (QC) protocols included field and laboratory blanks, duplicate samples, and measures to avoid external contamination (e.g., pre-cleaning equipment), as well as continuing GC-MS calibration verification using standard reference material (heptacosafluorotributylamine; Sigma Aldrich, Germany). Certified reference materials for the identified compounds were purchased from Sigma-Aldrich, Germany. Peak correlations have been done with the graphical help of the software AMDIS32 (Automated Mass Spectral Deconvolution and Identification System), XCalibur[™] (Thermo Fisher Scientific Inc., USA), and by hand. The limit of detection (LoD) was determined by signalto-noise ratio > 3. Blank corrections were not needed to be applied to the samples, as the examined pollutants did not appear in the blanks. While established quality control measures limit analytical inaccuracies, natural variations (e.g., [8, 35]) need to be considered.

Results

Inventory of flood-related contaminants

In the scope of this study, the non-polar pollutant inventories are divided into two primary categories—contaminants of the water-phase and sediment-associated contaminants. While all water-phase samples were collected from flooded households or basements, representing hotspots of flood-related damages, the flood-related sediments can be further subcategorized into samples from natural floodplains, urban areas subjected to high water stands and physical flood damages, and specific households or basements that can be identified as potential pollution hotspots.

Inventory of contaminants in the water phase

Severe flooding events, such as the 2021 flood, primarily trigger the release and remobilization of pollution through the aqueous phase (e.g., [19]). During the 2021 flood, several eyewitnesses and flood victims reported irritation of eyes and nasal mucosa, different smells in their basements (e.g., oil), and shimmering films flowing on top of the flood waters in their houses, which all can be indicators for (hazardous) pollution. Therefore, three household water samples (W1, W2, and W3) are screened for their pollution profile.

A total of 56 specific contaminants from three household water samples have been identified and inventorized (Table 2). The detected contaminants can be categorized based on their chemical applications into four groups: (A) personal care products, cosmetics, and odors; (B) technical additives; (C) surfactants and pharmaceuticals; and (D) other components.

Personal care products, cosmetics, and odors Within the personal care products, cosmetics, and odors group, seven organic compound classes of natural and synthetic origin have been identified in the water samples. Most dominant are alcohols, followed by terpenoids and esters, fatty acids, sterols, and phenylpropenes, as well as compounds specifically used as UV absorbers (Table 2; Fig. S1—supplement). As several organic substances linked to personal care products are of natural origins, such as oils and odors from plants, their environmental classification as pollutants is questionable. Nonetheless, their presence in the flood water samples indicates the release or mobilization of personal care products through flooding and physical damages.

Natural or plant-derived alcohols are important as essential oils in personal care products due to their preservative properties and fragrances. In total, seven alcohols were identified in the three water samples (Table 2): 2-phenylethanol, isoborneol, borneol, 4-*tert*butylcyclohexanol, terpinen-4-ol, hydroxycineole, and 1,3-diphenyl-2-propanol. The presence of natural organic alcohols in the 2021 floodwater samples but not in the sediment samples can be linked to their slight solubility in water. Most organic alcohols are biodegradable and are considered less environmentally harmful compared to their synthetic counterparts (e.g., [95]).

Terpenoids represent a diverse class of organic compounds derived from plants. For millennia, they have served as versatile ingredients in personal care products due to their fragrance, flavor, and therapeutic properties (e.g., antimicrobial, anti-inflammatory, and antioxidant properties; [3], and references therein). Four terpenoids have been identified in the flood water samples: camphor, carvone, aR-tumerone, and squalene (Table 2).

Other natural organic compounds identified include (1) the phenylpropene methyleugenol, which is primarily used in personal care products due to its flavoring and odor properties; however, in recent years, its addition to dietary products has been restricted due to its cancerogenic potential (e.g., [97, 113]); (2) the omega-6 fatty acid linoleic acid, which is industrially used as a dietary additive and in skin care products; and (3) the sterol stigmasterol, used as a dietary additive and personal care ingredient due to its hormone regulating properties (e.g., [5, 55]).

Artificially sourced UV absorbers are a common ingredient in personal care products, especially in sunscreen formulations and other skin care products (e.g., [72, Table 2 Occurrence of organic contaminants in the three water samples (W1, W2, and W3) from the Vicht and Inde rivers

Presonal case products, cosmetics and odorsAlconols2-Prenylethanol (PEA)CyllyD91,92XXXBoneolCyllyD95,110XXX4-tere ButylcyclobeanolCyllyD55,110XXXHydrogorineoleCyllyD57,81XXXHydrogorineoleCyllyD59,43XXXHydrogorineoleCyllyD99,43XXXTerpinen-AphoneCyllyD82,54XXXBoneolCyllyD83,110XXXTerpendsCyllyD83,110XXXSqualereCyllyD83,110XXXStatemeneCyllyD84,81XXXHydrogiamonata/hectioneCyllyD84,81XXXHydrogiamonata/hectioneCyllyD84,81XXXHydrogiamonata/hectioneCyllyD84,82XXXHydroppineTXXXXXHydroppineTXXXXXHydroppineTXXXXXHydroppineTXXXXXHydroppineCyllyD73,163XXXHydroppineCyllyDYXXXXHydroppineCyllyDYXXXXHydroppineCyllyD </th <th>Compound name</th> <th rowspan="2">Formula</th> <th rowspan="2">Sample <i>m/z</i></th> <th>W1</th> <th>W2</th> <th>W3</th>	Compound name	Formula	Sample <i>m/z</i>	W1	W2	W3
$ \frac{1}{2} 1$				Lab ID		
Personal care products, cosmetics and odors Alcohols 2-Precipiterianol (PEA) C.g.H.g.O 91,92 X X Bronnell C.g.H.g.O 95,111 X X Bronnell C.g.H.g.O 95,111 X X Bronnell C.g.H.g.O 95,110 X X Premper-A-cl C.g.H.g.O 77,811 X X Terpencid-cl C.g.H.g.O 77,811 X X Hydroxycincole C.g.H.g.O 95,81 X X Camphor C.g.H.g.O 87,81 X X X Canone C.g.H.g.O 87,81 X X X X Squalere C.g.H.g.O 87,81 X X X X Isoborpyl myristre C.g.H.g.O 83,82 X X X Isoporpyl myristre C.g.H.g.O 77,813 X X X Stoporpyl myristre C.g.H.g.O 77,8163 X X <				21/488	21/489	21/490
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Terpinen-4-ol Ci, HuO 71, 111 X X Hydroxycineole Ci, HuO 92, 91 X X Terpinen-4-ol Ci, HuO 92, 91 X X Terpinenols Ci, HuO 92, 91 X X Canone Ci, HuO 82, 54 X X aR-Turmerone Ci, HuO 83, 119 X X X Squalene Ci, HuO 83, 119 X X X Squalene Ci, HuO 83, 119 X X X Squalene Ci, HuO 83, 119 X X X Isobornyl acetate Ci, HuO 83, 82 X X X Isopropyl myinstare Ci, HuO 178, 163 X X X Hydrogenol Ci, HuO 178, 163 X X X Storols Ci, HuO 178, 163 X X X Tetry acids Ci, HuO 179, 144 X X<	4-tert-Butylcyclohexanol	C10H20	57.81		Х	Х
Hydroxycineole C ₁₁ H ₁₀ O ₂ 59,43 X 1.3-Diphenyl-2propanol C ₁₁ H ₁₀ O 92,91 X Camphor C ₁₀ H ₁₀ O 95,81 X X Caroone C ₁₀ H ₁₀ O 83,119 X X Squalene C ₂₀ H ₂₀ O 83,119 X X X Squalene C ₂₀ H ₂₀ O 83,102 X X X Esters Isobornyl acetate C ₂₀ H ₂₀ O, 83,102 X X X Isopropyl myfistate C ₁₀ H ₂₀ O, 43,60 X X X X Isopropyl myfistate C ₁₀ H ₂₀ O, 17,163 X X X Premyloropene U U X X X X Sterols U U Sterol St. X X Sterold C ₁₀ H ₂ O 17,43 X X X Premyloropene C ₁₀ H ₂ O,0 102,138 X X X Storo	Terpinen-4-ol	C10H10O	71, 111	Х	Х	
1.3-Diphenyl-2-propanol1.01.021.01.01.3-Diphenyl-2-propanol C_1H_1O 95, 81XXCamphor C_1H_1O 82, 54XXGarone C_1H_1O 83, 119XXSqualene C_2H_1O 83, 119XXSqualene C_1H_1O 95, 43XXEsters $C_{11}H_1O_2$ 43, 102XXIsopropyl palmitate $C_1H_1O_2$ 43, 60XXNethyl dhydrojasmonate/hedione $C_1H_1O_2$ 178, 163XXIsopropyl palmitate $C_1H_1O_2$ 178, 163XXMethyd ulydrojasmonate/hedione $C_1H_1O_2$ 178, 163XXIinoleic acid $C_1H_2O_3$ 67, 81XXSteroisSteroisXXXVir absorbers $C_2H_1O_0$ 55, 83XXXVir absorbers $Z_2H_1Tmethyl -1, 2-pentaneidol disoburyrate (TKIP)C_1H_1O_2101, 18XXZehrlinethyl -1, 3-pentaneidol disoburyrate (TKIP)C_1H_1O_2120, 138XXXVir absorbersZ_2H_1Tmethyl -1, 2-pentaneidol disoburyrate (TKIP)C_1H_1O_2125, 99XXZehrlinethyl -1, 3-pentaneidol disoburyrate (TKIP)C_1H_1O_212, 136XXXTrichord hylophashate (TCP)C_1H_1O_212, 10, 04XXXTriphenyl phosphate (TPP)C_1H_1O_212, 10, 04XXX$	Hydroxycineole	C10H20O2	59.43	X		
Terpends Terpends Carvone $C_1d_1_QO$ 95,81 X X Carvone $C_1d_1_QO$ 82,54 X aR-Turmerone $C_1d_1_QO$ 83,119 X X Squalene C_2d_1QO 69,81 X X X Squalene C_1d_1QO 83,129 X X X Isopropyl mytestate C_1d_1QO 83,82 X X X Isopropyl acetate C_1d_1QO 83,82 X X X Isopropyl anytistate C_1d_1QO 43,60 X X X Phenylpropene T T8,163 X X X Sterols T T8,163 X X X Sterols T T	1 3-Diphenyl-2-propanol	C15H150	92 91	X		
Campbool C _{in} H ₁₀ O 95,81 X X Carvone C _{in} H ₁₀ O 82,54 X aR-Turmerone C _{in} H ₂₀ O 83,119 X X Squalene C _{in} H ₂₀ O 83,119 X X Isobornyl acetate C _{in} H ₂₀ O, 83,129 X X Isobornyl acetate C _{in} H ₂₀ O, 83,02 X X Isobornyl acetate C _{in} H ₂₀ O, 83,02 X X Isopropyl myristate C _{in} H ₂₀ O, 43,002 X X X Isopropyl palmitate C _{in} H ₁₀ O, 178,163 X X X Fattry acids Lincleic acid C _{in} H ₂₀ O, 67,81 X X Stignasterol C _{in} H ₂₀ O, 67,81,80 X X X Pichnicia acidi Cisobarbers X X X X Stignasterol C _{in} H ₂₀ O, 71,43 X X X Actorylene (IOC) C _{in} H ₂₀ O, 71,43	Terpenoids	01511160	52, 51			
Carvone C, H ₁ , Q 25.50.1 N N Garvone C, H ₁ , Q 82, 54 X X aRTurmerone C, H ₂ , Q 83, 119 X X Squalene C, J ₂ H ₂ , Q 95, 43 X X X Sigoprop/ applicates C, H ₂ , Q ₂ 95, 43 X X X Isoporop/ applicates C, H ₂ , Q ₂ 43, 60 X X X Isoporop/ palmitate C, H ₂ , Q ₂ 43, 60 X X X Phenylpropene	Camphor	СНО	95 81	×	×	
Curron L $\Box_1 \phi_{12} O$ Δ_2 , Δ_2 Λ Squalene $C_{31}H_{30}O$ $69, 81$ X X X Squalene $C_{31}H_{32}O_3$ $83, 82$ X X Isobornyl acetate $C_{11}H_{22}O_3$ $83, 82$ X X X Isopropyl myristate $C_{11}H_{32}O_2$ $43, 60$ X X X Isopropyl paintate $C_{11}H_{32}O_2$ $78, 163$ X X X Phenylpropene U U adds X X X X Stignasterol $C_{10}H_{32}O_2$ $67, 81$ X X X UV absorbers $Z_{20}H_{40}O$ $55, 83$ X X X Technical additives (lasticizer, flame retardants, viscosity regulator, etc.) $Z_{24}H_{10}N_{10}O_2$ $Z_{14}H_{10}O_2$ X X X VU absorbers $Z_{24}H_{10}N_{10}O_2$ $Z_{14}, Z_{10}O_2$ $Z_{14}, Z_{10}O_2$ $Z_{14}, Z_{10}O_2$ X X Veltylbenzenesulfonamide (Uniplex IOR) $C_{10}H_{10}O_2$ $Z_{14}, Z_{10}O_2$ $Z_{14}, Z_{10}O_2$ <	Carvone	С Н О	82 54	~	X	
and utilitation $C_{1p}T_{2p0}$ $\delta_{2p}T_{1p0}$ $\delta_{2p}T_{1p0}$ $\delta_{2p}T_{1p0}$ Squalene $C_{2p}H_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p}T_{2p0}$ $\delta_{2p0}T_{2p0}$ $\delta_{2p0}T_{2p0}T_{2p0}$ $\delta_{2p0}T_{2p0}T_{2p0}T_{$		C L O	02, 34		×	
Signature Carthy C (9,8) X X X X X Esters Isobornyl acetate $C_1 \mu_1 \mu_2 O_2$ 95,43 X X Methyl dihydrojasmonate/hedione $C_3 \mu_1 \mu_2 O_2$ 43,102 X X X Isopropyl myristate $C_1 \mu_1 \mu_2 O_2$ 43,02 X X X Isopropyl apenitate $C_1 \mu_1 \mu_2 O_2$ 43,60 X X X Phenylpropene T T X X X Stigmasterol $C_{20} \mu_{40} O_2$ 67,81 X X X Stigmasterol $C_{20} \mu_{40} O_2$ 67,81 X X X Vu absorbers - - - X X X 2-4-Erinethyl-1,3-pentanediol disobutyrate (TXIB [®]) $C_1 \mu_3 D_0$ 71,43 X X X Vu absorbers - - - X X X 2-4-Erinethyl-1,3-pentanediol disobutyrate (TXIB [®]) $C_1 \mu_3 D_0 A_1$ 71,43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_$	Squalana	C ₁₅ H ₂₀ O	60.91	V	×	V
Isobomy Jacetate C ₁ H ₂ O ₂ 95,43 X Methyl dihydrojasmonate/hedione C ₁ H ₂ O ₂ 83,82 X Isoporopyl myristate C ₁ H ₂ O ₂ 43,102 X X Isoporopyl palmitate C ₁ H ₂ O ₂ 43,102 X X Phernylpropene X X X X Fatty acids	Squalene	C ₃₀ n ₅ 0	09, 81	~	~	~
Induction Cirptando 2 Git Pando 2	Esters		05 43		¥	
Methyl alrydrojasnonate/healone C ₁ H ₂₂ O ₂ 83, 82 X Isopropyl myristate C ₁ H ₂₄ O ₂ 43, 102 X X X Isopropyl palmitate C ₁ H ₁₄ O ₂ 43, 60 X X X Phenylpropene	Isobornyi acetate	$C_{12}H_{20}O_2$	95, 43		X	
Isopropyl myristate C ₁ ,H ₃ ,Q ₂ 43, 102 X X X Isopropyl palmitate C ₁₁ ,H ₃ ,Q ₂ 43, 60 X X X Phenylpropene C ₁₁ ,H ₁₄ ,Q ₂ 178, 163 X X X Fatty acids V X X X X X Sterols Sterols X X X X X VU absorbers C ₁₃ H ₂₂ O ₂ 67, 81 X X X X Octocrylene (C) C ₂₃ H ₄₈ O 55, 83 X X X X UV absorbers - - - X X X X X Coctorylene (C)C C ₂₃ H ₄₉ O 120, 138 X <td< td=""><td>Methyl dihydrojasmonate/hedione</td><td>C₁₃H₂₂O₃</td><td>83, 82</td><td></td><td>X</td><td>N/</td></td<>	Methyl dihydrojasmonate/hedione	C ₁₃ H ₂₂ O ₃	83, 82		X	N/
Isopropyl palmitate C ₁₉ H ₃₂ O ₂ 43, 60 X X Phenylpropene $(2_{19}H_{32}O_2)$ 178, 163 X X Fatty acids $(2_{19}H_{32}O_2)$ 67, 81 X X Inoleic acid $C_{19}H_{32}O_2$ 67, 81 X X Sterols 5 Sterols X X X UV absorbers $(2_{19}H_{32}O_3)$ 120, 138 X X X 2.4-Ethylhexyl salicylate (EHS) $C_{15}H_{32}O_3$ 120, 138 X X X Vabsorbers 2.2.4-Timethyl-1.3-pentanediol disobutyrate (TXIB [®]) $C_{16}H_{30}O_4$ 71, 43 X X X N-Ethyl-2-methylbenzenesulfonamide (Mispoury ate (TXIB [®]) $C_{10}H_{19}NO_5$ 91, 155 X X N-Ethyl-2-methylbenzenesulfonamide (Mispoury (TXIB [®]) $C_{10}H_{10}O_4$ 91, 155 X X N-Ethyl-2-methylbenzenesulfonamide (Mispoury (TXIB [®]) $C_{10}H_{10}O_4$ 92, 92 X X X Tristly lohosphate (TEP) $C_{10}H_{10}O_4$ 92, 92 X X X X Trighenyl phosphate (TPP)	Isopropyl myristate	C ₁₇ H ₃₄ O ₂	43, 102	X	Х	X
Phenylpropene Nethyleugenol C1 ₁ H ₁₄ O ₂ 178, 163 X X Fatty acids Linoleic acid C1 ₁₈ H ₃₂ O ₂ 67, 81 X X Sterols Sterols X X X UV absorbers Steroly Steroly Steroly X X 2-Ethylhexyl salicylate (EHS) C1 ₁₉ H ₃₂ O ₂ 204, 249 X X X Qctocrylene (OC) C ₂₄ H ₃₂ NO ₂ 204, 249 X X X Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) X X X X VLPhyl-2-methylbenzenesulfonamide (Uniplex 108) C ₁₀ H ₁₃ O ₂ A 71, 43 X X X N-Butylbenzenesulfonamide (NBSS or Uniplex 214) C1 ₁₀ H ₁₅ O ₄ P 91, 155 X X Trist2-chlorisopropyllphosphate (TCP) C ₉ H ₁₆ Cl ₃ O ₄ P 91, 155 X X Triphenyl phosphate (TPP) C ₁₀ H ₁₅ O ₄ P 326, 325 X X Trig-chlorosthyll phosphate (TCP) C ₁₄ H ₂ O ₄ P 43, 103 X X	Isopropyl palmitate	C ₁₉ H ₃₈ O ₂	43,60	Х		Х
Methyleugenol C ₁₁ H ₁₄ O ₂ 178, 163 X X Fatty acids - <td>Phenylpropene</td> <td></td> <td></td> <td></td> <td></td> <td></td>	Phenylpropene					
Fatty acids K X X Sterols Stignasterol C ₁₉ H ₃₂ O ₂ 67, 81 X X Stignasterol C ₂₉ H ₄₈ O 55, 83 X X X UV absorbers - - X X X 2-Ethylhexyl salicylate (EHS) C ₁₅ H ₂₂ O ₃ 120, 138 X X X Technical additives (plasticizers, flame retardants, viscosity regulators, etc. X X X X VL-hichex-nethylbenzenesulfonamide (Uniplex 108) C ₁₆ H ₃ O ₄ 71, 43 X X X N-Ethyl-2-methylbenzenesulfonamide (NBSS or Uniplex 214) C ₁₆ H ₁₅ O ₄ P 91, 155 X X X Trids2-chlorisopropyl)phosphate (TEP) C ₆ H ₁₅ O ₄ P 99, 155 X X X Trids2-chlorisopropyl)phosphate (TCPP) C ₉ H ₁₆ O ₄ O ₄ P 326, 325 X X X Trids2-chlorisopropyl)phosphate (TCPP) C ₉ H ₁₆ O ₄ P 31, 03 X X X Trids1-chloroethyl) phosphate (TCEP) C ₉ H ₁₂ O ₄ O ₇ 157, 29 <td>Methyleugenol</td> <td>C₁₁H₁₄O₂</td> <td>178, 163</td> <td></td> <td>Х</td> <td>Х</td>	Methyleugenol	C ₁₁ H ₁₄ O ₂	178, 163		Х	Х
Linoleic acid $C_{1g}H_{22}O_2$ $67, 81$ X X Sterols	Fatty acids					
Sterols $\sum_{2g} H_{4g} O$ 55, 83 X X IV absorbers $\sum_{2} Ethylhexyl salicylate (EHS) C_{15} H_{22} O_3 120, 138 X Octocrylene (OC) C_{2g} H_{27} NO_2 204, 249 X X Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) X X X 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®) C_{16} H_{30} O_4 71, 43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) C_{9} H_{18} NO_2S 91, 155 X X N-Butylbenzenesulfonamide (IMSS or Uniplex 214) C_{16} H_{15} O_4 P 99, 155 X X Tridyl phosphate (TEP) C_{9} H_{16} O_4 P 92, 59 X X X Triphenyl phosphate (TCP) C_{9} H_{16} O_4 P 326, 325 X X X Triacetin C_{9} H_{16} O_6 P 63, 249 X X X X Iried-cholosopropyl)phosphate (TCP) C_{16} H_{10} O_4 63, 77 X X X Iried-cholosopropyl)phosphate (TCP) C_{16} H_{10} O_4 463, 77 X X X <$	Linoleic acid	C ₁₈ H ₃₂ O ₂	67, 81		Х	Х
Stigmasterol $C_{29}H_{40}O$ 55, 83 X X UV absorbers	Sterols					
UV absorbers 2-Ethylhexyl salicylate (EHS) $C_{15}H_{22}O_3$ 120, 138 X 2-Ethylhexyl salicylate (EHS) $C_{24}H_{27}NO_2$ 204, 249 X X Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®) $C_{16}H_{30}O_4$ 71,43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_{9}H_{15}NO_2S$ 91, 155 X X N-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{16}H_{15}O_4P$ 99, 155 X X Triictyl phosphate (TEP) $C_{9}H_{18}O_2P$ 326, 325 X X X Triacetin $C_{9}H_{16}O_4$ 43, 103 X X X X Triethyl chroethyl) phosphate (TCEP) $C_{9}H_{12}O_4P$ 326, 325 X X X Triacetin $C_{9}H_{12}O_4P$ 326, 325 X X X Triethyl chroethyl) phosphate (TCEP) $C_{9}H_{12}O_4P$ 326, 325 X X Trigechin conspropyl)phosphate (TDCPP) $C_{9}H_{12}O_2$ 200, 107 X X If righyl chrof (6PF) $C_{19}H_{10}O_4$	Stigmasterol	C ₂₉ H ₄₈ O	55, 83	Х		Х
2-Ethylhexyl salicylate (EHS) $C_{15}H_{22}O_3$ 120, 138 X Octocrylene (OC) $C_{24}H_{27}NO_2$ 204, 249 X X Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) V X X 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®) $C_{16}H_{30}O_4$ 71, 43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_{9}H_{13}NO_2S$ 91, 155 X X N-Ethyl-benzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_2S$ 77, 141 X X Triethyl phosphate (TEP) $C_{9}H_{18}Cl_{0}A^{P}$ 92, 55 X X X Trijde-chlorosporpyl)phosphate (TCPP) $C_{9}H_{18}O_4P$ 93, 26, 325 X X X Triacetin $C_{9}H_{12}O_{10}A^{P}$ 157, 29 X X X Trific1,3-dichloroisopropyl)phosphate (TCPP) $C_{9}H_{12}Cl_{9}O_{7}P$ 157, 29 X X Irigacure® 184 $C_{12}H_{12}O_{2}$ 200, 107 X X X Phthalate $C_{10}H_{10}O_4$ 463, 77 X X X Dientyl phthalate (DMP)<	UV absorbers					
Octocrylene (OC) $C_{24}H_{27}NO_2$ 204, 249XXTechnical additives (plasticizers, flame retardants, viscosity regulators, etc.)XXXZ,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®) $C_{16}H_{30}O_4$ 71, 43XXXN-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_{9}H_{13}NO_2S$ 91, 155XXN-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_2S$ 77, 141XXTritelyl phosphate (TEP) $C_{6}H_{15}O_4P$ 99, 155XXTrijc2-chlorisopropyl)phosphate (TCPP) $C_{9}H_{16}O_4P$ 326, 325XXTriacetin $C_{9}H_{14}O_6$ 43, 103XXXTriacetin $C_{9}H_{14}O_6$ 43, 103XXXTrij (J-chlorosopropyl)phosphate (TCPP) $C_{9}H_{15}O_4P$ 63, 249XXTrij (J-chlorosthyl) phosphate (TCEP) $C_{9}H_{15}O_4P$ 75, 99XXXBisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107XXXIrgacure® 184 CDP $C_{19}H_{10}O_4$ 463, 77XXPhthalate DIP $C_{10}H_{10}O_4$ 463, 77XXXDisbutyl phthalate (DBP) $C_{16}H_{23}O_4$ 149, 177XXXDisbutyl phthalate (DBP) $C_{10}H_{10}O_4$ 463, 77XXXDisbutyl phthalate (DBP) $C_{16}H_{23}O_4$ 149, 177XXXDisbutyl phthalate (DBP) $C_{10}H_{20}O_4$ <td< td=""><td>2-Ethylhexyl salicylate (EHS)</td><td>C₁₅H₂₂O₃</td><td>120, 138</td><td></td><td></td><td>Х</td></td<>	2-Ethylhexyl salicylate (EHS)	C ₁₅ H ₂₂ O ₃	120, 138			Х
Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®) $C_{16}H_{30}O_4$ 71, 43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_9H_{13}NO_2S$ 91, 155 X N-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_2S$ 77, 141 X Triethyl phosphate (TEP) $C_6H_{15}O_4P$ 99, 155 X Tris(2-chlorisopropyl)phosphate (TCPP) $C_{19}H_{18}O_4P$ 326, 325 X Triacetin $C_9H_{14}O_6$ 43, 103 X X Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29 X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{12}G_3O_4P$ 63, 249 X X Bisphenol F (BPF) $C_{3}H_{12}O_2$ 200, 107 X X Irigacure® 184 $C_{10}H_{10}O_4$ 463, 77 X X Phthalate $C_{10}H_{10}O_4$ 463, 77 X X Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X Dimethyl phthalate (DBP) $C_{10}H_{12}O_4$ 149, 150 X	Octocrylene (OC)	C ₂₄ H ₂₇ NO ₂	204, 249	Х		Х
2,2,4-Trimethyl-1,3-pentanediol disobutyrate (TXIB®) $C_{16}H_{30}O_4$ 71,43 X X X N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_9H_{13}NO_2S$ 91,155 X N-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_2S$ 77,141 X Triethyl phosphate (TEP) $C_6H_{15}O_4P$ 99,155 X X Tris(2-chlorisopropyl)phosphate (TCPP) $C_{9}H_{18}G_3O_4P$ 125,99 X X X Triacetin $C_9H_{18}O_6A^P$ 326,325 X X X Triacetin $C_9H_{14}O_6$ 43,103 X X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_6H_{12}O_3Q_4P$ 63,249 X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{14}O_6$ 75,99 X X X Bisphenol F (BPF) $C_{13}H_{16}O_2$ 99,81 X X X Iragcure [®] 184 $C_{10}H_{10}O_4$ 463,77 X X X Dimethyl phthalate (DEP) $C_{10}H_{10}O_4$ 463,77 X X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ </td <td>Technical additives (plasticizers, flame retardants, viscosity regula</td> <td>ators, etc.)</td> <td></td> <td></td> <td></td> <td></td>	Technical additives (plasticizers, flame retardants, viscosity regula	ators, etc.)				
N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108) $C_9H_{13}NO_2S$ 91, 155 X N-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_2S$ 77, 141 X Triethyl phosphate (TEP) $C_6H_{15}O_4P$ 99, 155 X X Tris(2-chlorisopropyl)phosphate (TCPP) $C_9H_{18}Cl_3O_4P$ 125, 99 X X X Triphenyl phosphate (TPP) $C_{18}H_{15}O_4P$ 326, 325 X X Triacetin $C_9H_{14}O_6$ 43, 103 X X X Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29 X X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{12}Cl_3O_4P$ 63, 249 X X X Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X X X Irgacure [®] 184 $C_{10}H_{10}O_4$ 463, 77 X X X Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X X Dibutyl phthalate (DBP) $C_{10}H_{14}O_4$ 149, 177 X X X Disobutyl phthalate (DBP) $C_{16}H_{22}O_4$	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (TXIB®)	C ₁₆ H ₃₀ O ₄	71, 43	Х	Х	Х
N-Butylbenzenesulfonamide (NBSS or Uniplex 214) $C_{10}H_{15}NO_{2}S$ 77, 141 X Triethyl phosphate (TEP) $C_{6}H_{15}O_{4}P$ 99, 155 X Tris(2-chlorisopropyl)phosphate (TCPP) $C_{9}H_{18}Cl_{3}O_{4}P$ 125, 99 X X X Triphenyl phosphate (TPP) $C_{18}H_{15}O_{4}P$ 326, 325 X X X Triacetin $C_{9}H_{14}O_{6}$ 43, 103 X X X Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_{7}$ 157, 29 X X Tri(2-chloroethyl) phosphate (TCEP) $C_{6}H_{12}Cl_{3}O_{4}P$ 63, 249 X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_{9}H_{16}O_{2}P$ 75, 99 X X Bisphenol F (BPF) $C_{13}H_{12}O_{2}$ 200, 107 X X Irgacure® 184 $C_{19}H_{10}O_4$ 463, 77 X X Phthalate Dimethyl phthalate (DMP) $C_{16}H_{12}O_4$ 463, 77 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Disbutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 157	N-Ethyl-2-methylbenzenesulfonamide (Uniplex 108)	C ₉ H ₁₃ NO ₂ S	91, 155			Х
Triethyl phosphate (TEP) $C_6H_{15}O_4P$ 99, 155 X Tris(2-chlorisopropyl)phosphate (TCPP) $C_9H_{18}Cl_3O_4P$ 125, 99 X X X Triphenyl phosphate (TPP) $C_{18}H_{15}O_4P$ 326, 325 X X X Triacetin $C_9H_{14}O_6$ 43, 103 X X X Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29 X X Tri(2-chloroethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ 63, 249 X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ 75, 99 X X Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X X Irgacure® 184 $C_{19}H_{10}O_4$ 463, 77 X X Phthalates Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 57 X X X Disobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X	N-Butylbenzenesulfonamide (NBSS or Uniplex 214)	C ₁₀ H ₁₅ NO ₂ S	77, 141			Х
Tris(2-chlorisopropyl)phosphate (TCPP) $C_9H_{18}Cl_3O_4P$ 125, 99XXXXTriphenyl phosphate (TPP) $C_{18}H_{15}O_4P$ 326, 325XXXTriacetin $C_9H_{14}O_6$ 43, 103XXXTriethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29XXTri(2-chloroethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ 63, 249XXXTris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ 75, 99XXXBisphenol F (BPF) $C_{13}H_{10}O_2$ 200, 107XXXIrgacure® 184 $C_{10}H_{10}O_4$ 463, 77XXXPhthalates $C_{10}H_{10}O_4$ 463, 77XXXDimethyl phthalate (DMP) $C_{16}H_{22}O_4$ 149, 177XXXDibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 57XXXDisobutyl phthalate (DIP) $C_{16}H_{22}O_4$ 149, 57XXXDiscotut phthalate (DIP) $C_{16}H_{22}O_4$ 149, 57XXXDisobutyl phthalate (DIP) $C_{16}H_{22}O_4$ 149, 57XXXDiscotut phthalate (DIP) $C_{16}H_{20}O_4$ 140, 167<	Triethyl phosphate (TEP)	C ₆ H ₁₅ O ₄ P	99, 155			Х
Triphenyl phosphate (TPP) $C_{18}H_{15}O_4P$ $326, 325$ XTriacetin $C_9H_{14}O_6$ $43, 103$ XXTriethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ $157, 29$ XTri(2-chloroethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ $63, 249$ XXTris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ $75, 99$ XXBisphenol F (BPF) $C_{13}H_{12}O_2$ $200, 107$ XXIrgacure [®] 184 $C_{13}H_{16}O_2$ $99, 81$ XXPhthalates V V V XXDimethyl phthalate (DMP) $C_{10}H_{10}O_4$ $463, 77$ XXDibutyl phthalate (DBP) $C_{16}H_{22}O_4$ $149, 150$ XXXDisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 57$ XXXDiisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 157$ XXXDiisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 157$ XXXDiisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 157$ XXX	Tris(2-chlorisopropyl)phosphate (TCPP)	C ₉ H ₁₈ Cl ₃ O ₄ P	125, 99	Х	Х	Х
Triacetin $C_9H_{14}O_6$ 43, 103 X X Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29 X X Tric(2-chloroethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ 63, 249 X X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ 75, 99 X X X Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X X X Irgacure® 184 $C_{13}H_{16}O_2$ 99, 81 X X X Phthalates X X X X Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X X Dibutyl phthalate (DEP) $C_{16}H_{22}O_4$ 149, 177 X X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 157 X X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 157 X X X	Triphenyl phosphate (TPP)	C ₁₈ H ₁₅ O ₄ P	326, 325		Х	
Triethyl citrate (TEC or Uniplex 80) $C_{12}H_{20}O_7$ 157, 29 X Tris(1,3-chlorosethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ 63, 249 X X Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ 75, 99 X X Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X X Irgacure® 184 $C_{13}H_{16}O_2$ 99, 81 X X Phthalates U U X X Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 177 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X X	Triacetin	C ₉ H ₁₄ O ₆	43, 103	Х		Х
Tri(2-chloroethyl) phosphate (TCEP) $C_6H_{12}Cl_3O_4P$ $63, 249$ XXTris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ $75, 99$ XXBisphenol F (BPF) $C_{13}H_{12}O_2$ $200, 107$ XXIrgacure® 184 $C_{13}H_{16}O_2$ $99, 81$ XXPhthalates $C_{10}H_{10}O_4$ $463, 77$ XXDimethyl phthalate (DMP) $C_{10}H_{10}O_4$ $463, 77$ XXDibutyl phthalate (DBP) $C_{16}H_{22}O_4$ $149, 177$ XXDibutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 57$ XXXDiisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 57$ XXXDiisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 157$ XXX	Triethyl citrate (TEC or Uniplex 80)	C ₁₂ H ₂₀ O ₇	157, 29			Х
Tris(1,3-dichloroisopropyl)phosphate (TDCPP) $C_9H_{15}Cl_6O_4P$ 75, 99 X X Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X Irgacure® 184 $C_{13}H_{16}O_2$ 99, 81 X X Phthalates Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X Dimethyl phthalate (DEP) $C_{12}H_{14}O_4$ 149, 177 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X X	Tri(2-chloroethyl) phosphate (TCEP)	C ₆ H ₁₂ Cl ₃ O ₄ P	63, 249	Х		Х
Bisphenol F (BPF) $C_{13}H_{12}O_2$ 200, 107 X Irgacure® 184 $C_{13}H_{16}O_2$ 99, 81 X X Phthalates $C_{10}H_{10}O_4$ 463, 77 X X Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X X Diethyl phthalate (DEP) $C_{12}H_{14}O_4$ 149, 177 X X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X X	Tris(1,3-dichloroisopropyl)phosphate (TDCPP)	C ₉ H ₁₅ Cl ₆ O ₄ P	75, 99	Х	Х	
Irgacure® 184 $C_{13}H_{16}O_2$ 99, 81 X X Phthalates Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X Dimethyl phthalate (DEP) $C_{12}H_{14}O_4$ 149, 177 X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 157 X X	Bisphenol F (BPF)	C ₁₃ H ₁₂ O ₂	200, 107		Х	
Phthalates C10H10O4 463,77 X Dimethyl phthalate (DMP) C12H14O4 149,177 X Dibethyl phthalate (DBP) C16H22O4 149,150 X X Dibotyl phthalate (DIBP) C16H22O4 149,57 X X Diisobutyl phthalate (DIBP) C16H22O4 149,57 X X	Irgacure [®] 184	C12H14O2	99, 81	Х		Х
Dimethyl phthalate (DMP) $C_{10}H_{10}O_4$ 463, 77 X Diethyl phthalate (DEP) $C_{12}H_{14}O_4$ 149, 177 X Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149, 150 X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X Diisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149, 57 X X	Phthalates	15 10 2	,			
Distribution $C_{10}H_{10}O_4$ $100 F_1$ $100 F_1$ Diethyl phthalate (DEP) $C_{12}H_{14}O_4$ $149, 177$ XDibutyl phthalate (DBP) $C_{16}H_{22}O_4$ $149, 150$ XXDisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ $149, 57$ XXDiscostyl phthalate (DIOP) $C_{16}H_{22}O_4$ $149, 167$ XX	Dimethyl phthalate (DMP)	C10H10O4	463 77		х	
Dibutyl phthalate (DBP) $C_{16}H_{22}O_4$ 149,150XXXDisobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149,57XXXDiscostyl phthalate (DIOP) $C_{16}H_{22}O_4$ 149,167XXX	Diethyl phthalate (DEP)	$C_{12}H_{14}O_{4}$	149 177		X	
Disobutyl phthalate (DIBP) $C_{16}H_{22}O_4$ 149,57XXDiscontrul phthalate (DIOP) $C_{16}H_{22}O_4$ 149,167XX	Dibutyl phthalate (DBP)	$C_{12}H_{22}O$	149 150	х	X	Х
Discontryl phthalate (DIOP) $C \perp O$ 140 167 V V V	Diisobutyl obthalate (DIRP)	C16 ¹ 122 ⁰ 4	149 57	~	X	X
	Diisooctyl phthalate (DIOP)	C24H2004	149 167	Х	X	X

Table 2 (continued)

Compound name	Formula	Sample <i>m/z</i>	W1	W2	W3
			Lab ID		
			21/488	21/489	21/490
Bis(2-ethylhexyl) phthalate (DEHP)	C ₂₄ H ₃₈ O ₄	149, 167	Х	Х	Х
Dioctyl isophthalate (DOIP)	C ₂₄ H ₃₈ O ₄	261, 167	Х	Х	
Surfactants and pharmaceuticals					
Surfactants and bleach					
2,4,7,9-Tetramethyl-5-decin-4,7-diol (Surfynol [®] 104 or TMMD)	C ₁₄ H ₂₆ O ₂	109, 43	Х		Х
N,N,N',N'-Tetraacetylethylenediamine (TAED)	C ₁₀ H ₁₆ N ₂ O ₄	43, 72		Х	Х
Diethylene glycol monododecyl ether (Laureth-2)	C ₁₆ H ₃₄ O ₃	57, 45	Х	Х	
Drugs					
Myosmine	$C_9H_{10}N_2$	118, 146		Х	
Caffeine	C ₈ H ₁₀ N ₄ O ₂	194, 109		Х	Х
Pharmaceuticals					
N-Benzylformamide (NBFA)	C ₈ H ₉ NO	135, 134	Х		
2-Phenyl-2-propanol	C ₉ H ₁₂ O	43, 121	Х	Х	
Cholesterol	C ₂₇ H ₄₆ O	43, 55	Х		Х
Other compounds					
Phenol	C ₆ H ₆ O	94, 66	Х	Х	
Benzothiazole	C ₇ H ₅ NS	135, 108		Х	Х
Indole	C ₈ H ₇ N	117, 90	Х	Х	
1-Phenoxypropan-2-ol	C ₉ H ₁₂ O ₂	94, 77	Х	Х	
Acetophenone	C ₈ H ₈ O	105, 77	Х		
Oxyphenalon (rheosmin or 4-frambinone)	C ₁₀ H ₁₂ O ₂	107, 164	Х		
Verbenone	C ₁₀ H ₁₄ O	107, 91	Х		
2-Methylbenzothiazole	C ₈ H ₇ NS	149, 108		Х	
Cannabinol, TMS derivative	C ₂₄ H ₃₄ O ₂ Si	367, 368	Х	Х	

Compound name, formula, m/z and occurrence in the three respective samples are given

73]). In this study, two UV absorbers have been identified, namely octocrylene (OC) and 2-ethylhexyl salicylate (EHS) (Table 2). While both compounds possess only low toxicities to humans and most mammals [76], their high persistency and toxicity to aquatic life (e.g., coral bleaching) pose a significant environmental risk (e.g., [20, 65]). In recent years, regulatory bodies in some regions have started to restrict or ban the use of certain UV absorbers, including octocrylene and 2-ethylhexyl salicylate, to mitigate their impact on aquatic environments (e.g., [2, 23]).

Technical additives (plasticizers, flame retardants, viscosity regulators, etc.) Various compounds with specific applications and physicochemical properties have been identified among the technical additives. The most dominant components based on their occurrence across all three water samples are plasticizers and substances used in plastic production (e.g., flame retardants, viscosity regulators, etc.; Fig. S2—supplement). For decades, plasticizers have been an environmental concern (e.g., [15, 18, 98, 109], and references therein). Some plasticizers are known to leach from plastic products into the environment, posing risks to ecosystems and human health [6, 69, 75]. Plasticizers, particularly phthalate-based, have been documented to intensively contribute to water and air pollution (e.g., [16, 98, 112]) and can accumulate in sediments (e.g., [37, 93, 117]).

The most frequent plasticizers identified in the water samples are dimethyl phthalate (DMP), diethyl phthalate (DEP), dibutyl phthalate (DBP), diisooctyl phthalate (DIOP), bis(2-ethylhexyl) phthalate (DEHP), and dioctyl isophthalate (DOIP) (Fig. 3; Fig. S2—supplement). Their ubiquitousness in everyday products and building materials (e.g., [11, 86]) is reflected in the presence of diverse congeners in the flood water samples. In addition to urban sources, the release of phthalate from the flooded industrial areas along the Vicht and Inde rivers (e.g., Stolberg and Eschweiler) must be considered for the 2021 flood. Generally, phthalates cause environmental stability in combination with health hazard effects, such as



Fig. 3 GC–MS chromatograms of phthalates (*m*/*z* 149) in both fractions of water sample W2. Fraction F1 containing diethyl phthalate (DEP), dibutyl phthalate (DBP), diisooctyl phthalate (DIOP). In fraction F2 the phthalates dimethyl phthalate dimethyl phthalate (DMP), diisobutyl phthalate (DIBP), dioctyl isophthalate (DOIP) were identified. In both fraction the degradation product phthalic acid ester (PAE) was found

endocrine disruption, reproductive toxicity, and developmental issues [64, 69]. In recent years, there has been increased monitoring, scrutiny, and regulation of phthalate use in certain applications (e.g., [53]). Other compounds of technical and industrial origin detected in the water samples comprise compounds with various properties. Non-phthalate-based plasticizers include 2,2,4-trimethyl-1,3-pentanediol diisobutyrate (TXIB[®]), N-ethyl-2-methylbenzenesulfonamide (Uniplex 108), and N-butylbenzenesulfonamide (NBBS or Uniplex 214). The identified compounds triethyl phosphate (TEP), tris(2-chlorisopropylphosphate (TCPP), and triphenyl phosphate (TPP) exhibit additional flameretardant properties along with their plasticizing capabilities. Plasticizers with additional attributes include triacetin (stabilizing properties), triethyl citrate (TEC) or Uniplex 80; used in coatings or as food/pharmaceutical additive, tri(2-chloroethyl phosphate (TCEP); flame-retardant and viscosity regulating properties, and tris(1,3-dichloroisopropylphosphate (TDCIPP); flameretardant properties and pesticide characteristics. Furthermore, Bisphenol F (BPF), a popular precursor to produce plastics and epoxy resins, was identified in the water samples. Its presence suggests flood-related mobilization of organic compounds from industrial sources and local plastic sources. Likewise, the presence of Irgacure[®] 184, a photoinitiator for coatings and adhesives, connotes the release of industrial effluents and the mobilization of contaminants from industrial areas along the flood-affected river catchment.

Surfactants and pharmaceuticals The urban effluent indicators detected in the flood water samples comprised different specific substances that can be cat-

egorized as surfactants, pharmaceuticals, and drugs (Table 2). All three groups pose different risks to the environment and human health.

Among the surfactants and bleach compounds are three substances, namely 2,4,7,9-tetramethyl-5-decin-4,7-diol (traded as Surfynol[®] 104 or TMMD), N,N,N',N'tetraacetylethylenediamine (TAED), and diethylene glycol monododecyl ether (traded as Laureth-2) (Table 2; Fig. S3-supplement). TMMD is used in industrial applications as surfactants (e.g., [41, 68]), but also as an additive in pesticides (e.g., glyphosate [54]). TAED is commonly used as a bleach activator in detergents (e.g., [48, 84]). TAED is typically removed during wastewater treatment [39], however, due to TAED's biodegradability, its products might have a greater ecotoxicological impact on the environment than TAED itself (e.g., [21]). Laureth-2 is an emulator and washing-active substance of the laureth family of surfactants. It is not inherently harmful to humans, as it is frequently used in washing lotions and other personal care products (e.g., [31, 51]), however, once laureth-2 enters the aquatic ecosystems, it raises environmental concerns. Such anionic surfactants have been reported to have negative effects on fish and microorganisms (e.g., [10, 17]).

Pharmaceuticals, drug-related compounds, and their human excretory products are frequently found in urban effluents and can even reach aquatic environments after wastewater treatment [1], and references therein. In the flood water samples, three pharmaceutical intermediates and two drug-related substances have been identified (Table 2). The detected compounds *N*-benzylformamide (NBFA), 2-phenyl-2-propanol, and cholesterol are intermediate substances in the chemical and pharmaceutical industry. They are often linked to pharmaceutical synthesis and have been documented in urban effluents (e.g., [7]). The drug-related compounds are caffeine and myosmine (closely related to nicotine). They have been documented in urban effluents and are afflicted with significant environmental concerns [58], and references therein; [57, 81]. These compounds indicate flood-related urban effluents from households or industrial effluents from flood-affected chemical plants (e.g., in Stolberg: Grünethal GmbH, West Pharmaceutical Services GmbH & Co. KG, and others) entering the aqueous environment and entrapment in urban households and basements.

In general, the presence of biodegradable surfactants, pharmaceutical substances, and drugs in the water samples from the 2021 flood indicates the leakage or flooding of sewage systems (Fig. 1A; e.g., [108, 114]—this issue). Most of the identified compounds would be removed during wastewater treatment under normal circumstances. Nonetheless, due to the interruption as a result of physical damages to sewer systems, the flooding of public and household sewers, and the inundation of sewage treatment plants along the Vicht–Inde catchment (e.g., WWTP Stolberg-Steinfurt & Eschweiler), the flood-induced release of untreated urban effluents into urban areas and the environments needs to be considered.

Other components (aromatics, ketones, etc.) Other compounds identified in the three water samples encompass aromatic derivatives (e.g., phenol, benzothiazole—vulcanization inhibitor, indole, 1-phenoxypropan-2-ol) that might be derived from road runoff, ketones (e.g., acetophenone, oxyphenalon), terpenoids with insect control properties (e.g., verbenone), and intermediate substances used for chemical synthesis (reactants, stabilizers, etc.) and industrial applications (e.g., 2-methylbenzothiazole, cannabinol, TMS derivative).

Inventory of sediment-bound contaminants

Along with physical damages, sediments constitute the most evident remnant of flooding events. Sediments of the 2021 flood exhibit a mixture of sand, silt, clay, debris, and organic material. The grain size composition and the organic matter content are the two controlling factors that govern contaminant transport and determine a sediment's capability and capacity to accumulate pollutants (e.g., [35, 61]). Generally, with smaller grain sizes, pollution loads increase, with the most abundant pollution linked to organic-rich clays (e.g., [56, 74]). All flood sediments sampled for this study are composed primarily of silt with various amounts of debris (e.g., building material and fragments, plastics, and household items, particularly in and downstream of urban areas, e.g., Fig. 1D; for grain size data see [110]-this issue. Some floodplain sediments exhibit a higher content of the sand fraction.

Flood sediments reflect a multitude of sedimentary and associated pollution sources based on release, erosion/remobilization of old burdens and legacy pollution, transport, and deposition in sinks or when the transport capacity is decreasing with lower flow speeds (e.g., [19]). By the nature of their deposition, flood sediments can be distinguished into two main categories along the Vicht– Inde catchment: (1) floodplain deposits that are deposited naturally with lowering and slowing water masses, and (2) urban or household deposits that are entrapped and deposited in man-made sinks.

Non-target screening of the 12 analyzed sediment samples from floodplains (n=5), urban areas (n=5), and households (n=2) revealed a multitude of different environmentally contaminant groups, such as petrogenics, urban effluent and wastewater compounds, chlorinated industrial compounds, pesticides, and less environmentally common substances.

Petrogenic and pyrogenic pollution The homologues series of $C_{29}-C_{35}$ hopane stereoisomers (Table 3) has been identified in all sediment samples. The series is characterized by a predominance of C₃₀ over C₂₉, and C_{31} hopanes with a less dominant presence of C_{32} - C_{35} hopanes (Fig. 4A; Fig. S4-supplement). Ubiquitously identified in all sediments are polycyclic aromatic hydrocarbons (PAHs; Table 3). Among the detected congeners are the EPA 16 PAHs: naphthalene (m/z=128), acenaphthylene (m/z=152), acenaphthene (m/z=154), fluorene (m/z=166), phenanthrene (m/z=178), anthracene (m/z = 178), fluoranthene (m/z = 202), pyrene (m/z = 202), benz[a]anthracene (m/z=228), chrysene (m/z=228), benzo[b]fluoranthene (m/z=252), benzo[k]fluoranthene (m/z=252), benzo[a]pyrene (m/z=252), dibenzo[a,h] anthracene (m/z = 278), benzo[g,h,i]perylene (m/z = 276), and indeno[1,2,3-cd]pyrene (*m*/*z*=276) (Fig. 4B; Fig. S4 supplement).

The simultaneous presence of hopanes and PAHs in sediments is indicative of petrogenic and pyrogenic pollution. Geohopanes are diagenetic products of biohopanes and are commonly derived from petroleum and petroleum products (e.g., fossil fuels; [80]). Hopanes are resistant to degradation, rendering them long-term pollution risks and generally suitable indicators of petrogenic pollution (e.g., [40]). PAHs, on the other hand, are a group of organic compounds with multiple fused aromatic rings, predominantly produced during incomplete combustion of organic matter [115]. Both groups pose significant environmental and health risks due to their prevalence, persistence, toxicity, and potential carcinogenicity (e.g., [4, 78]). The specific PAH composition can serve as a key for identifying their sources, such as the composition present in the samples, which indicate
 Table 3
 Occurrence of specific organic contaminants in floodplain sediments, urban sediment and household sediments from samples along the Vicht and Inde rivers

Compound group	Compound name		Formula	m/z
Petrogenic compounds				
Hopanes	α-C ₂₉ hopane		C ₂₉ H ₅₀	191
	C ₂₉ Ts hopane		C ₂₉ H ₅₀	191
	β -C ₂₉ hopane		C ₂₉ H ₅₀	191
	α-C ₃₀ hopane		C30H52	191
	β-C ₃₀ hopane		C30H52	191
	22S-C ₃₁ hopane		C ₃₁ H ₅₄	191
	22R-C ₃₁ hopane		C ₃₁ H ₅₄	191
	22S-C ₃₂ hopane		C32H56	191
	22R-C ₃₂ hopane		C ₃₂ H ₅₆	191
	22S-C ₃₃ hopane		C33H28	191
	22R-C ₃₃ hopane		C33H58	191
	22S-C ₃₄ hopane		C34H60	191
	22R-C ₃₄ hopane		C34H60	191
	22S-C ₃₅ hopane		C35H62	191
	22R-C ₃₅ hopane		C35H62	191
Polycyclic aromatic hydrocarbons (PAHs)	Naphthalene		C ₁₀ H ₈	128
	Acenaphthylene		C ₁₂ H ₈	152
	Acenaphthene		C ₁₂ H ₁₀	154
	Fluorene		C ₁₃ H ₁₀	166
	Phenanthrene		C ₁₄ H ₁₀	178
	Anthracene		C ₁₄ H ₁₀	178
	Fluoranthene		C ₁₆ H ₁₀	202
	Pyrene		C ₁₆ H ₁₀	202
	Benz[a]anthracene		C ₁₈ H ₁₂	228
	Chrysene		C ₁₈ H ₁₂	228
	Benzo[b]fluoranthene		C ₂₀ H ₁₂	252
	Benzo[k]fluoranthene		C ₂₀ H ₁₂	252
	Benzo[a]pyrene		C ₂₀ H ₁₂	252
	Dibenzo[a,h]anthracene		C ₂₂ H ₁₂	276
	Benzo[g,h,i]perylene		C ₂₂ H ₁₂	276
	Indeno[1,2,3-cd]pyrene		C ₂₂ H ₁₂	276
Urban effluents and wastewater indicators				
Linear alkyl-benzenes (LABs)	Phenyldecane		C ₁₆ H ₂₆	91, 105
	Phenylundecane		C ₁₇ H ₂₈	91, 105
	Phenyldodecane		C ₁₈ H ₃₀	91, 105
	Phenyltridecane		C19H32	91, 105
Technical and industrial pollutants				
Polychlorinated biphenyls (PCBs)	Pentachlorobiphenyl (Cl ₅ -PCB)		C ₁₂ H ₅ Cl ₅	326
	Hexachlorobiphenyl (Cl ₆ -PCB)		C ₁₂ H ₄ Cl ₆	360
	Heptachlorobiphenyl (Cl ₇ -PCB)		C ₁₂ H ₃ Cl ₇	396
Diisopropyl-naphthalenes (DIPNs)	Several isomers		C ₁₆ H ₂₆	197, 212
Alkylsulfonic acid phenylesters	Tetradecyl-ASE	Mesamoll®	C ₂₀ H ₃₄ O ₃ S	94
	Pentadecyl-ASE		C ₂₁ H ₃₆ O ₃ S	94
	Hexadecyl-ASE		C ₂₂ H ₃₈ O ₃ S	94
	Heptadecyl-ASE		C ₂₃ H ₄₀ O ₃ S	94
Triglyceride	Triacetin		C ₉ H ₁₄ O ₆	43

Identified compound groups are differentiated into petrogenic compounds (hopanes; polycyclic aromatic hydrocarbons—PAHs), urban effluents and wastewater indicators (linear alkylbenzenes—LABs), as well as technical and industrial pollutants (polychlorinated biphenyls—PCBs; diisopropylnaphthalenes—DIPNs; alkylsulfonic acid phenylesters—ASE/Mesamoll[®])



Fig. 4 Petrogenic pollutants hopanes and polycyclic aromatic hydrocarbons. **A** Chromatograms (m/z = 191) of homologue series of C₂₉–C₃₅ hopane stereoisomers in representative floodplain (F3) urban (U1) and household (H1) sediments. **B** Chromatograms of detected PAHs: naphthalene (Nap; m/z = 128), acenaphthylene (Acy; m/z = 152), acenaphthene (Ace; m/z = 154), fluorene (FI; m/z = 166), phenanthrene (Phe; m/z = 178), anthracene (Ant; m/z = 178), fluoranthene (Flu; m/z = 202), pyrene (Pyr; m/z = 202), benz[a]anthracene (B[a]A; m/z = 228), chrysene (Chr; m/z = 228), benzo[b] fluoranthene (B[b]F; m/z = 252), benzo[a]pyrene (B[a]P; m/z = 252), dibenzo[a,h]anthracene (DBA; m/z = 278), benzo[q,h,i]pervlene (B[dhi]P; m/z = 276), and indeno[1,2,3-cd]pyrene (Ind; m/z = 276)

oil spills, anthropogenic discharges, or remobilization of legacy pollution.

Urban effluents and wastewater indicators In the studied flood sediments, the indicative substance group linear alkylbenzenes (LABs) associated with sewage-derived hydrophobic pollution were identified. LABs are a class of organic compounds that find significance in various industrial applications, particularly as detergents and synthetic lubricants. They are characterized by linear alkyl chains attached to a benzene ring. Four LAB congeners (C_{10} —phenyldecanes, C_{11} —phenylundecanes, C_{12} —phenyldodecanes and C₁₃—phenyltridecanes; m/z=91/105) have been detected across the samples (Fig. 5A; Fig. S5-supplement). Released into the environment since the 1960s, LABs are a byproduct of linear alkylbenzene sulfonate (LAS), a key ingredient in many household detergents [26, 43]. Despite their widespread use, LABs are environmental pollutants of concern, particularly in aquatic ecosystems (e.g., [25, 43, 50]). The release of LABs into water bodies typically occurs through domestic wastewater discharges or industrial effluents (e.g., [46]). To qualitatively evaluate this discharge and to estimate the treatment status of wastewater discharges, the *I/E* ratio of the C_{12} homologs proposed by Takada and Ishiwatari [101] can be consulted. It is a ratio of internal to external isomers of LABs, where the external substituted isomers are more readily biodegraded [50, 101].

Generally, low I/E ratios suggest untreated sewage to be released into the environment [50]. More specifically, Takada and Eganhouse [102] concluded I/E ratios between 0.7–0.75 to originate from raw untreated wastewater, encompassing ranges between 0.52 and 0.86 from primarily treated wastewater and ratios ranging from 2 to 7.3 to originate from secondarily treated wastewater. In addition, Isobe et al. [50] postulated I/E ratio ranges of 0.7–1.2 for untreated wastewater. For the purpose of this study, the given framework by Takada and Eganhouse



detected LAB congeners (C₁₀—phenyldecanes, C₁₁—phenylundecanes, C₁₂—phenyldodecanes, and C₁₃—phenyltridecanes). **B** Illustration of *I/E* ratios for each sampling point. Ranges for wastewater treatment level according to Takada and Eganhouse [102] and Isobe et al. [50]: *I/E* of 2.0–7.3 = secondary treated wastewater, *I/E* of 0.52–0.86 = primary treated wastewater; *I/E* of 0.7–0.75 = raw untreated wastewater; and *I/E* of 0.7–1.2 = untreated wastewater

[102] was used for the interpretation of the I/E ratio (Fig. 5B; see supplementary Table S1). Results show that the I/E ratio of LABs in most urban and household sediments reflect a primary treatment of wastewater that affected the samples. Similar do the rural floodplain samples F2, F3, and F4 located in the lowlands with lower flood-impacts reflect the influence of primary treated wastewater. Distinct outlier here is the household sample H2 which indicates contamination by untreated wastewater, likely linked to the flooding of the wastewater treatment plant in Eschweiler or local input by broken sewage systems. Similar are the floodplain samples F1 located in the valley-confined upland connected to severe destruction of critical infrastructure including sewage systems, and the sample F5 which is located downstream at the confluence with the Rur, likely reflecting urban influence by the flooded wastewater treatment plant in Düren.

The hydrophobic characteristics and persistency of LABs favor their accumulation in river and floodplain

sediments (e.g., [46, 50, 104]). Previously to the 2021 flood, LAS have been detected in the surface waters of the Rur catchment [89], and LABs were detected in the floodplains of the Rur River [92], in which the Vicht–Inde catchment flows into. In the case of the 2021 flood, damages to infrastructure, breakage, leakage, and flushing of sewers and pipes (Fig. 1A), as well as the remobilization of old burdens, need to be considered as major pollution sources.

Technical and industrial pollutants Two substance groups classified as technical or industrial contaminants have been detected in the flood sediments from the Vicht–Inde catchment. These are polychlorinated biphenyls (PCBs) and diisopropylnaphthalenes (DIPNs) (Fig. S5—supplement).

PCBs are man-made compounds that do not naturally occur and were widely used in industrial applications between the 1930s and 1970s (e.g., [27, 77]). Their use

encompasses industrial and technical applications, such as electrical insulation, plasticizers in lacquer, coolants, and hydraulic fluids (e.g., [27]). The synthesis of PCBs entails the chlorination of biphenyls, conducted in the presence of a catalyst, resulting in over 209 known congeners [12, 49, 105]. This chemical transformation, characterized by the stepwise addition of chlorine atoms to biphenyl, creates PCB congeners with varying degrees of chlorination. This study identified three PCB congeners (Cl_5 —pentachlorobiphenyl, Cl_6 —hexachlorobiphenyl, and Cl_7 —heptachlorobiphenyl).

PCB mixtures were traded in Germany as Clophen since the 1930s (Bayer AG) or imported as Askarel, Aroclor (both Monsanto Chemical Company, USA), or Pyralene (Prodelec, France) [77, 105, 107]. International agreements are in place since the early 2000s to reduce environmental exposure to persistent organic pollutants (POP [13]). For PCBs specifically, a ban has been ratified by the Stockholm Convention on Persistent Organic Pollutants, which came into force in 2004 [106]. PCBs are still ubiquitous in the global environment despite the bans and restrictions on production and usage [13]. Their constant presence can be linked to old burdens, and only $\sim 30\%$ of countries are on track to hold up the agreed-upon requirement to manage PCB legacies by 2028 (Stockholm [70, 100]). In Germany, 30-50% of PCB legacies were mismanaged, and by 2013, 12,000 t PCBs in open application (in buildings/construction, transformers, electrical wiring, etc.) remained and contributed to 7-12 t of PCBs released into the environment annually [111]. As a consequence of their high persistency, lipophilicity, and low vapor pressure, PCBs accumulate in soils and sediments, from where they have a path into the food chain [77]. In the context of the 2021 flood, old burdens (e.g., [96]) must be considered sources for PCBs in the Vicht-Inde catchment based on the physical damages and destruction, particularly in the uplands of the Vicht valley.

DIPNs are a class of organic contaminants with a broad field of industrial applications, including usage as solvents, lubricants (e.g., [79]), and additives in various products (e.g., food packaging material—[116], plant growth regular, and paper production—[38]). Furthermore, DIPNs are used as substitutes for PCBs. In the environment DIPNs are commonly reported since the late 2000s [38] and due to their resistance to biodegradation, DIPNs are becoming a raising environmental concern, despite their comparatively low toxicity (e.g., [47]). For the flood-samples contamination by DIPNs can be linked to industrial sources, similar to PCB emission sources. The vast destruction in the study area, the flooding of industrial sites, and flushing out of sewage systems all contribute to the release and distribution of

DIPNs throughout the river catchments. This is further supported, as Schwanen et al. [92]—this issue, have also identified DIPNs in the Rur river into which the Vicht and Inde rivers flow. These downstream observations are likely linked to industrial emission sources along the Vicht and Inde catchments where most of the destructive flood-impacts took place.

Noteworthy other contaminants Within the sediment samples, different individual contaminants have been detected. Among them, the most noteworthy are alkyl-sulfonic acid phenylesters, carbazole, triacetin, and chlorobenzenes.

Non-phthalate-based plasticizers have been used more frequently in recent decades; however, some of these compounds are also afflicted with environmental concerns. One group that has been used since the 1960s as an extender or full replacement for dimethyl phthalate or extender in PVC production are alkylsulfonic acid phenylesters (ASE; [44]). In this study, various ASE congeners, combined marketed as Mesamoll®, have been detected in all samples. In total, four homologous groups of ASEs (C₁₄—tetradecyl derivatives, C₁₅—pentadecyl derivatives, $\rm C_{16}-hexadecyl$ derivatives, and $\rm C_{17}-heptadecyl$ derivatives; Fig. 6C) have been identified in the sediments. Through the past two decades, few studies provided evidence for the widespread distribution of Mesamoll® in the environment, as well as the ability to adsorb and accumulate in sediments (e.g., [7, 34, 36, 83, 94]). Mesamoll[®] pollution in the Rur catchment, to which the Vicht-Inde catchment contributes, has previously been documented by Schwanen et al. [92].

Another non-phthalate-based plasticizer identified in the flood sediment is triacetin (Table 3). Its presence in the sediments is noteworthy, as triacetin is water soluble and is a prevailing component in the aqueous samples. Beyond triacetin's utilization as a plasticizer, it is commonly used in other industrial applications, including as a solvent and additive in the production of food, pharmaceuticals, and personal care products [32, 33]. While it is not typically considered a significant environmental pollutant, certain aspects, such as its acute toxicity, raise environmental concerns (e.g., [63]). However, information on its potential long-term effects on ecosystems is limited.

Discussion

Environment-specific contaminant characteristics, sources of flood-induced pollution, and hotspots

For the qualitative pollution assessment of the 2021 flood, the complex interplay between flood dynamics and contaminant behavior necessitates a nuanced understanding of how diverse environmental settings shape the nature



Fig. 6 Chromatograms of technical and industrial pollutants. **A** Chromatogram polychlorinated biphenyls (PCBs) represented by PCB congeners pentachlorobiphenyl (Cl₅; m/z=326), hexachlorobiphenyl (Cl₅; m/z=360), and heptachlorobiphenyl (Cl₇; m/z=396); **B** chromatogram of diisopropylnaphthalenes (DIPNs; m/z=212) with several isomers; **C** Chromatogram of alkylsulfonic acid phenylesters (Mesamoll[®], m/z=94) represented by C₁₄-tetradecyl, C₁₅-pentadecyl, C₁₆-hexadecyl, and C₁₇-heptadecyl derivates

and extent of flood-related pollution release, remobilization, and distribution. Such insights are fundamental for devising targeted remediation strategies and fostering resilience in the face of the increasing unpredictability of extreme weather and flood events. Therefore, a distinction is made between two domains that affect pollution throughout the Vicht–Inde catchment under investigation during the flood: the aqueous and sediment phases.

Characteristics and sources of aqueous pollution

The extensive release and remobilization of pollutants driven by flood-induced destruction is reflected in the water samples exhibiting a diverse range of individual contaminants, indicative of the flood-related pollution from localized direct (point-) sources and diffuse catchment-encompassing sources. On the contrary, the water masses are transported downstream much faster than sediments or suspension loads. Thus, the effective residence time of aqueous pollution is relatively short (~ hours). This residence time can be prolonged in urban areas where circumstances allow water to pond for extended periods (days to weeks) or flood water is trapped in households, basements, or garages. Thereby, households not only act as sinks for aqueous pollution, but also as a yet rarely considered pollution source.

All water samples originate from urban areas. However, the external and environmental conditions vary between the three sampling locations. Sample W1 from Stolberg is collected in an area that experienced severe damages, erosion, and flooding (Fig. 1). Pollution by urban and industrial effluents can be directly linked to damaged sewage systems and flooding of households, and larger industrial plants. Particularly, the industrial complex located upstream of Stolberg along the Vicht experienced damages and flooding, likely causing the release or remobilization of pollutants. Some of the industries affected include copper, copper alloy, and brass processing (Aurubis Solberg GmbH & Co.; William Prym Holding GmbH), as well as personal care, perfume, and detergent production (Dalli-Werke GmbH & Co.; s. Oliver Cosmetics GmbH; Mäurer & Wirtz GmbH & Co. KG). Nonetheless, the impact of flood-derived industrial effluents is reflected in the water samples.

The water samples W2 and W3 were collected from basements in downstream areas in Eschweiler, where the physical damages of the flood were less severe, and the prevalent damages occurred from high water levels. The two samples differ from one another in terms of contaminant diversity. While sample W3 exhibits the lowest diversity in contaminants, sample W2 shows a high diversity in contaminants. As the damages to the households were relatively low (compared to upstream areas of Stolberg) and only limited industrial areas are in the vicinity or direct upstream areas of the water samples W2 and W3, their specific aqueous pollution inventories can be linked to in situ sources. Households and basements themselves provide plentiful sources of organic contaminants. Most German houses have all critical infrastructure (water/sewage pipes, electricity, oil heating systems, etc.) in the basement. Furthermore, basements are frequently used for storage and laundry. All these factors play an important role during the inundation of flood water, as numerous in situ sources for personal care products, detergents, phthalates, petrogenics, and other compounds are given on an individual basis. In the larger

scope of floods, such local sources for aqueous pollution have been neglected. However, the environmental and health impact in such localized hot spots may surpass the overall pollution in a river's catchment and must be considered in post-flood remediation efforts.

Sources of sediment-associated floodplain pollution

Floodplain sediments are often referred to as "*a waterbody's memory*" (e.g., [14, 28, 42, 45]) reflecting a long history of floods, land-use change, and the discharged pollution. This is also true for the floodplains affected by the 2021 flood, as they recorded the flood itself in the form of sedimentary remnants and extensive floodrelated sediment-associated pollution throughout the Vicht–Inde catchment. This pollution may be converted into legacy pollution once the 2021 flood sediments are incorporated into the respective floodplain's sedimentary archive, posing a long-term risk to local communities and ready to be remobilized during future flood events.

The collected and analyzed floodplain sediments show location-specific characteristics, thus the studied floodplains along the Vicht–Inde catchment distinguish into (A) the floodplains upstream of urban agglomerations (F2); (B) downstream floodplains in the immediate vicinity of urban agglomerations (F1 and F3); and (C) river restoration floodplains significantly downstream of urban agglomerations (F3–F5).

The floodplain sample F2 from upstream areas of Stolberg at the Inde River presents the lowest overall pollution qualitatively. While this area has been significantly affected by the 2021 flood, direct sources for the emission of sediment-associated pollutants are limited at site F2 and upstream.

At the sample location, F1 from the Vicht floodplain downstream of the severely affected town of Zweifall and upstream of Stolberg, a high abundance of pollutants reflects the localized release. Particularly, petrogenic pollution from hopanes and PAHs is prevalent in sample F1. Due to the flooding, physical damages, and severe destruction in the valley-confined uplands of the Vicht catchment till the Vicht–Inde confluence, a multitude of potential point sources need to be considered. Foremost is the destruction of oil tanks, heating systems, and vehicles, releasing pollution from upstream urban areas onto the floodplain sinks. Other sources, such as run-off, remobilization, or diffuse pyrogenic sources, may also have played a role in the 2021 flood.

Three samples from river restoration floodplains have been taken downstream of the city Eschweiler (F3), along the rerouting "Neue Inde" outside of the lignite mine Inden (F4), and the Inde–Rur confluence (F5). While these floodplains are aimed to be restored to near-natural environments through rehabilitation efforts, they also present significant sinks for pollution-associated flood sediments. In contrast to the naturally and artificially channelized river sections of the valley-confined upland and through the urban agglomerations, the lateral extension of the river corridor in restoration zones offers vast retention areas in the shape of floodplains and riparian areas for the flood water to reclaim during an event. In these areas, the flow speed was drastically reduced, even during the 2021 flood event, leading to the increased deposition of sediments and associated pollution (e.g., [62]). Schulte et al. [88] documented for floodplains of the "Neue Inde" an enrichment of heavy metals in allochthonous flood sediments prior to the 2021 flood. Similar observations can be made for the organic pollutants, despite a lack of local pollution sources, the level of present contaminants is notable.

In general, the sediment-associated pollution evident in the 2021 flood deposits from floodplains is substantial, thereby raising long-term environmental concerns. The presence of persistent and ecologically hazardous groups of contaminants, exemplified by PCBs, PAHs, and plasticizers (DIPNs, Mesamoll[®]), has the potential to attenuate rehabilitation efforts within zones designated for river restoration.

Sources of sediment-associated pollution in urban environments and households

The 2021 flood greatly affected urban areas like Stolberg, Eschweiler, and villages along the Vicht-Inde catchment. Substantial quantities of flood-derived sediments from upstream regions and local erosion processes (Figs. 1 and 7) are deposited in these urban areas. The consequences were particularly severe, with several hundred houses and critical infrastructure (e.g., SAH hospital in Eschweiler) succumbing to flooding. The floodwater reached up to the first floor in the valley-confined uplands, while the lowlands witnessed predominantly flooding of basements resulting in distinct sediment deposition patterns. This led to different pollution profiles between outdoor urban surfaces (e.g., roads, sidewalks, and squares) and indoors deposits (e.g., basements). The sediment-laden floodwaters infiltrated buildings, particularly basements, where they were confined, allowing sediments to settle out of suspension (e.g., Fig. 7). This spatial confinement and settling process may lead to variations in the pollution patterns between flood sediments. Notably, samples collected from households and basements displayed a higher complexity in their pollutant congeneric distribution. The differences in pollution levels suggest that local sources within buildings may play a dominant role in influencing the overall quality and quantity of sedimentassociated pollution.

Pollution hotspots vs. wash-out effects

The inventory of aqueous and sediment-associated contaminants in deposits from various affected environments by the 2021 flood emphasizes the presence of pollution hot spots and wash-out effects across the Vicht–Inde catchment. At first glance, these may seem conflicting in the same event, but the environmental divergence between urban areas and floodplains causes drastic differences in fluvial and flood-related pollution dynamics.

One of the main contributors to localized hotspot pollution in urban areas is the fast discharge of flood water during the 2021 event (e.g., [62]) that enabled the observed scale of physical damages, erosion, and transport of large debris and sediments. These effects are amplified in the upland valley-confined and channelized urban river sections. Here, the pronounced effects of lateral erosion led to the impairment of infrastructure (e.g., bridges) and buildings (e.g., [62]). Through damages to industrial areas, housing quarters, and urban infrastructure (e.g., sewage treatment plants, waste disposal sites, etc.), as well as the erosion of legacy contaminants (e.g., from mining areas), flood-induced sediment-associated pollution is released or remobilized. The nature of urban environments creates numerous areas where flood water discharge velocities can decrease and sediments, alongside their pollution load, accumulate. In the outdoors, wider areas (roads, squares, etc.) and confined places (backyards, alleys, etc.) emerge as sedimentation and pollution hotspots (Figs. 1 and 7). This is further supported by the organic pollution inventory of both water and sediment samples indicating that indoor areas of buildings may be considered as flood-induced pollution hotspots.

Within the confines of houses and buildings, externally released or remobilized pollutants (e.g., from industrial plants or old burdens) associated with the sediment-rich flood water are transported into buildings where they meet and mix with contaminants of in situ pollution sources activated by the inundating flood water (Fig. 7). In situ sources include but are not limited to building infrastructure (plumbing, heating), building materials (PVC pipes, cable insulations, etc.), everyday items (personal care products, laundry, and cleaning agents), gardening chemicals (fertilizers, pesticides, herbicides), home improvement measures (paint, oils, lubricants, rust preventative, etc.), electronic equipment (photocopier ink, computers, etc.), and many more (Fig. 7). The presented pollution inventory reflects these diverse contamination sources. Short-term health hazards to disaster relief workers, volunteer helpers and residents may originate from flood waters and sediments in houses. However, longterm hazards may arise from pollutants infiltrating into



Fig. 7 Photo plate of flood-related damages and pollution sources along the Vicht and Inde rivers. A Damages to a road, erosion of the sidewalk and piping infrastructure in the industrial areas at Zweifaller Straße (L238) in Stolberg. Photo—courtesy of Tristan Lothmann. B Unknown white foam oozing from sewer in the aftermath of the flood. The foam is likely linked to the release of household and industrial surfactants. Photo—courtesy of Tristan Lothmann. C Flooded basement with in situ pollution sources from home improvements items (e.g., oils, lubricants, etc.). Photo—courtesy of Tristan Lothmann. D Flooded garage and workshop with numerous potential in situ pollution sources. Photo—courtesy of Tristan Lothmann. E Flooded office room covered in a thin layer of mud. In situ pollution sources from everyday electronic items and office supplies. Located in a municipal office building at Willy-Brand Platz in Stolberg. Photo—courtesy of Tristan Lothmann. F Muddy flood deposits on basement stairs in Stolberg. First responders and relief workers needed to wear improvised protective gear against hazardous pollution. Photo—courtesy of Tristan Lothmann

walls, furniture, and other household items. Apart from mold, hazardous aerosols (e.g., [29]) and dust (e.g., [110]—this issue) can emanate from the evaporation of organic contaminants over extended periods, creating long-term health risks for the local population.

In the larger scope of floods, concerns arising from pollution, particularly localized pollution, have been neglected in the past despite the imminent environmental and health impact in such localized hotspots, which may surpass the overall pollution in a river's catchment. In future disaster relief strategies, local pollution must be considered as a short-term hazard to first responders and a long-term hazard to residents. Appropriate actions need to be developed for future post-flood remediation efforts.

In contrast to the pollution hotspots, it is imperative to acknowledge that a significant proportion of the flood-associated pollution has likely been transported downstream along the Rur (as documented by Schwanen et al. [92]) and Meuse rivers. The phenomenon of washing-out is often overlooked in flood analyses (e.g., [7, 66]).

The activation of pollution sources is most pronounced in the early stages of a flood ("first flush"), coinciding with the peak of physical damages and flood expansions [67]. Subsequently, these pollution sources are drained, and the released contaminants are transported downstream (unless entrapped) throughout the duration of the flood, culminating in their eventual sediment-associated deposition at later stages of the flood event, when water current velocities subside below the minimum transport threshold. Furthermore, it is pertinent to consider that certain flood deposits may undergo erosion during subsequent flood pulses. The 2021 flood event, for instance, witnessed the occurrence of at least 2-3 distinct flood pulses recorded by gauges in Mulatshütte (Vicht), Kornelimünster, and Eschweiler (Inde), further complicating the dynamics of sediment-associated pollution transport and deposition. Collectively, these mechanisms give rise to a pollution wash-out phenomenon in unconfined river sections, notably floodplains (e.g., [7]). This occurrence presents a potential concern, particularly given that numerous post-flood investigations commonly focus on surveying "unaltered" floodplains, viewing them as archives for flood-induced pollution. However, this approach may inadvertently lead to a systematic underestimation of the actual extent of contamination release and the pollution potential associated with catastrophic floods. Consequently, relying (mostly) on floodplains for post-flood assessments neglects the intricate dynamic nature of flood-derived pollution, resulting in an incomplete understanding of the complex interplay between pollution release, remobilization, transport, deposition, and their broader environmental implications across various timescales.

Conclusions

By inventorying the non-polar organic contamination in water and sediment samples, this study provides a comprehensive qualitative overview of the intricate pollution dynamics during the 2021 flood. Thereby, this study offers valuable insights into (A) diversity in pollutant presence across different environments (floodplains, urban, and household); (B) the multifaceted circumstances of pollutant release, remobilization, and transport; and (C) emphasizing the role of local conditions (sustained damages, pollution hotspots and wash-out effects) and pollution sources to gain a better understanding of the true nature of flood-induced pollution.

It is imperative to acknowledge pollution hotspots and wash-out effects in flood pollution assessments for a more accurate evaluation of the impact of floods on environmental pollution. Further, this study emphasizes the importance of addressing the immediate and long-term consequences of pollution resulting from natural flood disasters, exemplified by the 2021 flood in Germany. This pollution may be converted into legacy pollution once the 2021 flood sediments are incorporated into the respective floodplain's sedimentary archive, posing a long-term risk to local communities and ready to be remobilized during future flood events. The potential conversion of contaminants emitted or remobilized by the 2021 flood into legacy pollution, underscores the need for targeted remediation efforts to mitigate both short-term and longterm environmental impact and health hazards arising from flood-associated pollution. In future disaster relief strategies, local pollution must be considered as a shortterm hazard to first responders and a long-term hazard to residents. Appropriate actions need to be developed for future post-flood remediation efforts.

In the larger scope of floods, concerns arising from pollution, particularly localized pollution, have been neglected in the past despite the imminent environmental and health impact in such localized hotspots, which may surpass the overall pollution in a river's catchment. Recognizing the transitory nature of catastrophic floods and their associated pollution potential becomes paramount, particularly in times of increasing environmental and pollution-related challenges exacerbated by climatedriven extreme events. Acknowledging this is crucial to gaining a more profound understanding of pollution sources and distribution processes, thereby enabling the development of effective environmental monitoring actions and strategies to protect water quality, preserve ecosystems, and promote human well-being. The qualitative results of this study are the basis for a specific quantitative analysis of pollution concentrations and variations across the catchments and the development of suitable future strategies.

Supplementary Information

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Supplementary Material 1.

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Author contributions

PB, JS, and KR were involved in planning and conducting all aspects of the research and laboratory work. KR organized the field work and all authors participated in the field survey immediately after the flood in 2021. Laboratory analyses were conducted under the supervision of JS and PB. PB and JS administered and performed the analyses and data interpretation. KR provided additional research data on the flood deposits. PB wrote the initial manuscript draft. All authors reviewed and edited the manuscript before submission.

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Availability of data and materials

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Declarations

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Competing interests

The authors declare that they have no competing interests.

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